



# Lithium-Ion Battery Designer

## About the Lithium-Ion Battery Designer Application

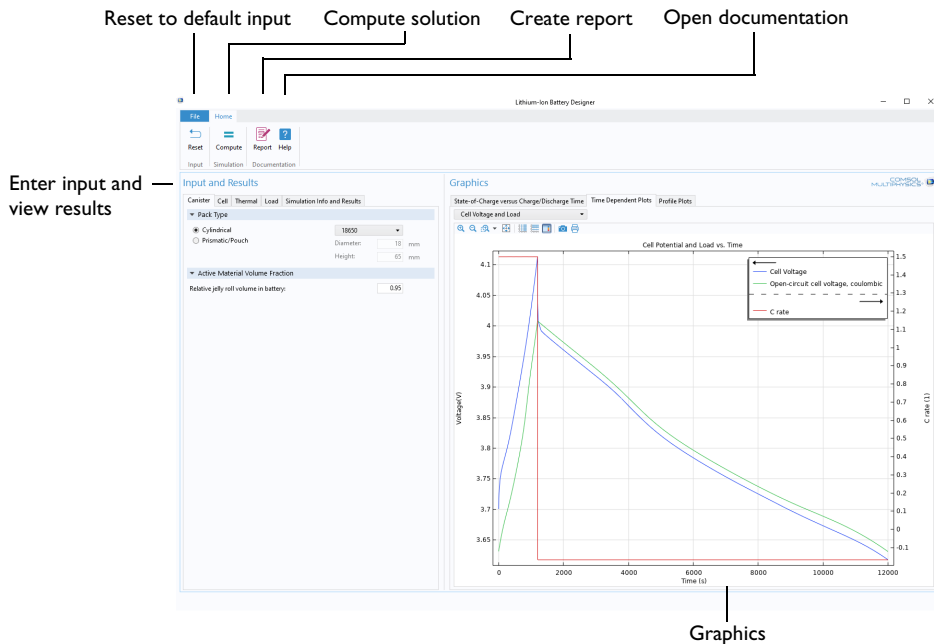
This application can be used as a design tool to develop an optimized battery configuration for a specific application. The application computes the capacity, energy efficiency, heat generation and capacity losses due to parasitic reactions of a lithium-ion battery for a specific load cycle.

In the application you can change various battery-design parameters, such as the geometrical dimensions of the battery canister, the thicknesses of the different components (separator, current collectors and electrodes), the positive electrode material, and the volume fractions of the different phases of the porous materials.

The load cycle is a charge-discharge cycle using a constant current load, which may be different for the charge and discharge stages.

The application also computes the battery temperature (assuming an uniform internal battery temperature), based on the generated heat and the thermal mass. Cooling is defined using an ambient temperature parameter and a heat transfer coefficient.

The figure below shows the application's user interface (UI).



To use the app, do as follows:

- 1 Set the geometrical dimensions of the battery canister in the **Canister** tab. This will define the volume, and also the cooling area of the cell.
- 2 Define the battery cell parameters in the **Cell** tab. The application will automatically set the thickness of the negative electrode to match the positive capacity + the provided excess capacity. The resulting theoretical capacity (at an infinitely slow charge/discharge rate) for the set of input parameters is shown at the bottom of this tab.
- 3 The thermal mass (the density and the heat capacity) of the battery are set in the **Thermal** tab. Here you also specify the ambient temperature and the heat transfer coefficient which is used for cooling the cell. The cooled area is calculated automatically, based on the settings in the **Canister** tab.
- 4 In the **Load** tab you specify the charge-discharge cycle. The battery will start by charging from the lower SOC limit, and switch to discharge when the upper SOC limit is reached. The C-rates are based on the theoretical maximum capacity of the battery. If you choose to set the charge and discharge times, this means that the application will automatically set the battery load currents to match the provided times and the theoretical maximum capacity of the battery.
- 5 Click the **Compute** button to solve the model equations.
- 6 Once the model equations are solved, you may review various numerical values in the **Simulation Info and Results** tab. Various plots, based on the simulation, can be reviewed under the **Time Dependent Plots** and the **Profile Plots** tabs on the right. You may also generate a report by pressing the **Report** button on the ribbon.

### *Strategies for Battery Design*

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There are several aspects of battery performance that may be interesting when studying a battery system. You may want to maximize the energy output, for a specified charge-discharge cycle, given a number of design constraints such as a minimum cycle energy efficiency, a maximum temperature rise, and maximum relative capacity losses due to parasitic reactions. This simulation application is intended for such studies.

After running such a study, you may also want to go through the following check-list:

- Are the design constraints fulfilled?
- Am I using all available capacity in both electrodes?
- Is the current distribution uniform?
- What are the electrode potentials? Is the battery close to plating or gassing?

### **MAXIMIZING ENERGY OUTPUT**

The energy density of a battery is a combination of many factors. Typically you want to maximize the average cell voltage, the used capacity, and the volume of electrode material in the cell, as well as optimize the balance between the two electrodes. The following guidelines may apply:

- Go for a high-voltage positive electrode material (but be aware of gassing!)
- Lower the negative excess host capacity
- Increase electrode thicknesses
- Increase the electrode volume fractions
- Use more available capacity by increasing the SOC cycling window.

### **MINIMIZING ENERGY LOSSES (AND TEMPERATURE RISE)**

The energy losses (and heat sources) occur as a result of ohmic losses in the electrolyte and electrode phases (Joule heating), activation losses in the charge-transfer reactions and concentration gradients in the cell. The following measures decrease the losses:

- Decrease electrode thicknesses
- Decrease electrode volume fractions
- Decrease the cell current by decreasing the SOC cycling window.

### **HOW TO AVOID PLATING**

Lithium plating occurs for electrode potentials below 0 V vs Li/Li<sup>+</sup>. This can typically occur on the negative electrode for high SOC during charge, when the graphite host material is saturated and unable to intercalate more lithium. The following measures mitigate plating issues:

- Lower the upper SOC limit
- Increase the negative electrode host capacity
- Use a thinner electrode with less material to get a uniform current distribution.

### **HOW TO AVOID GASSING**

Gassing occurs at high potentials. To avoid gassing, you can do the following:

- Change to a positive electrode material with a lower open circuit voltage
- Decrease the upper SOC limit of the positive electrode
- Use a thinner electrode with less material to get a uniform current distribution.

### MODEL DEFINITION

The model embedded in the application is based on a transient formulation of the equations for the conservation of chemical species, current, and charge in a Li-ion battery.

The model consists of the following components:

- Positive porous electrode (different materials may be selected in the application): active material, electronic conductor, and binder.
- Negative graphite porous electrode: active material, electronic conductor, and binder.
- Porous separator
- Electrolyte: 1.2 M LiPF<sub>6</sub> in EC:EMC (3:7 by weight).

The geometry consists of three domains the negative graphite electrode, the separator, and the positive electrode.

Concentrated electrolyte theory is used to define the ion transport, and the lithium intercalation and the transport of solid lithium in the negative and positive electrode particles is modeled by Fick's law in an extra (pseudo) dimension. The equations describing the fundamental cell chemistry are documented in "1D Isothermal Lithium-Ion Battery" tutorial in the Battery Design Module Application Library. The model is an extended version of the so-called Newman model.

### PARASITIC REACTIONS

Lithium plating occurs irreversibly on the negative electrode when the electrode potential is negative to Li/Li<sup>+</sup>.

$$i_{\text{loc, Plating}} = i_{0, \text{Plating}} \left( e^{\frac{\eta F}{2RT}} - e^{-\frac{\eta F}{2RT}} \right) \quad \eta < 0 \quad (1)$$

Gassing occurs on irreversibly the positive electrode according to

$$i_{\text{loc, Gassing}} = i_{0, \text{Gassing}} e^{\frac{\eta F}{2RT}} \quad (2)$$

The gassing is hence always present on the positive electrode. However, due to the exponential relationship it will be negligible if the potential of the positive electrode is kept low enough.

## ENERGY BALANCE EQUATION

The embedded model also solves for a temperature dependent variable, using the following lumped energy balance equation:

$$\rho C_p \frac{dT}{dt} = Q_{\text{tot}} - Ak(T - T_{\text{amb}}) \quad (3)$$

where  $\rho$  is the lumped density, and  $C_p$  the heat capacity of the battery.  $Q_{\text{tot}}$  is the sum of all heat sources, integrated over the whole battery cell.  $A$  is the cooling area and  $k$  the corresponding heat transfer coefficient between the battery and the ambient temperature  $T_{\text{amb}}$ . The initial temperature when the simulation starts is equal to the ambient temperature.

## Reference

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1. M. Doyle, J. Newman, A.S. Gozdz, C.N. Schmutz, and J.M. Tarascon, “Comparison of Modeling Predictions with Experimental Data from Plastic Lithium Ion Cells,” *J. Electrochem. Soc.*, vol. 143, no. 6, pp. 1890–1903, 1996.

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**Application Library path:** Battery\_Design\_Module/Applications/  
li\_battery\_designer

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